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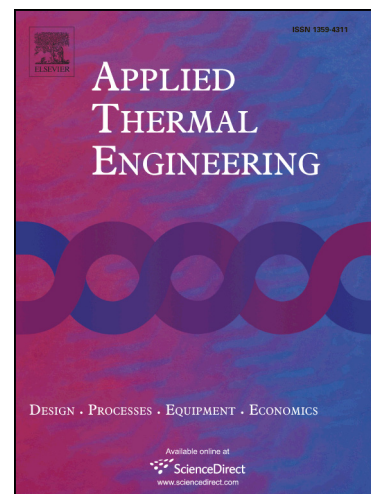
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**OPTIMAL SYNTHESIS OF MULTIPERIOD HEAT EXCHANGER
NETWORKS: A SEQUENTIAL APPROACH**

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ABSTRACT

Heat exchanger network (HEN) synthesis is an important research field in industrial processes. It is possible to minimize utilities usage as well as pollutant emissions by an optimal HEN synthesis. In multiperiod HENs, the same heat transfer devices must be able to operate under different operating conditions. The synthesis of multiperiod HEN can be formulated as an optimization problem. In the present paper it is used a sequential approach to solve the problem of synthesizing multiperiod HEN, considering heat capacities and stream temperatures variations into different operation periods. In this approach, multiperiod HEN synthesis is decomposed into three sequential steps, considering three optimization models. The novelties of the proposed approach are a modification in a well-known superstructure from the literature, with the inclusion of new by-pass streams, and an improvement in the NLP model of the third step. Two benchmark literature examples are studied and the obtained results prove the approach applicability, showing better values and network topologies.

Keywords: heat exchanger networks, optimization, multiperiod operation, mathematical programming.

1. INTRODUCTION

Heat exchanger network (HEN) synthesis has been treated as an optimization problem with mathematical programming being used to solve it. The main objective is to minimize the total annual cost (TAC). The HEN can operate in multiple periods, in which the heat transfer devices should be able to accept changes in the operating conditions (inlet and outlet process streams temperatures, flowrates or composition).

Although mathematical programming dominates recently published papers in the field of synthesis of multiperiod HENs, the earliest papers were published by Linnhoff and co-workers and were based on pinch analysis. Linnhoff and Kotjabasakis [1] and Kotjabasakis and Linnhoff [2] introduced important concepts like downstream paths and sensitivity tables, aiming to identify the effect of disturbances on the controlled variables. A trade-off among energy, capital cost, and flexibility was used to synthesize multiperiod HENs, and a strategy was presented to reduce the cost of fouling in HENs. Ravagnani and Módenes [3] used flexibility analysis to achieve a HEN design able to operate in different periods, which was achieved with algorithmic adaptations of a base case HEN, aiming the lowest global costs. The base case was designed using Pinch Analysis.

Floudas and Grossmann [4] presented the first study using mathematical programming to solve the problem of the flexible HENs. In that work, the authors considered pre-specified changes in the supply and target temperatures and in the flowrates during finite periods. They proposed a sequential procedure, composed by two steps: the minimization of the utilities cost for each period and the minimization of the number of heat transfer units. In that way, the work was an application of the linear programming (LP) and an extension of the Mixed Integer Linear Programming (MILP) models of Papoulias and Grossmann [5], solved separately for each period of operation. The final HEN structure was then derived manually for each sub-network, using information on heat duties and matches, obtained from the MILP problem solution. Since two problems (LP and MILP) are solved sequentially, this approach became known in the literature as a sequential one, with each optimization problem being applied to each step of the procedure. In sequential approaches for the synthesis of HENs, operated or not in multiple periods, different optimization problems are solved and it is supposed that the first problem to be solved takes precedence over the following one. Furthermore, the

solution found for a problem serves as input to the next problem. A sequential approach has as major advantage the fact that simpler optimization problems are solved sequentially, when compared to a simultaneous approach, which solves only one optimization problem for the HEN synthesis.

In the following year, Floudas and Grossmann [6] presented an improved version of their previous approach [4], generating automatically the multiperiod HEN configuration, with the use, in a third step (the first two steps were those of their previous work), of the Non Linear Programming (NLP) model of Floudas *et al.* [7]. A superstructure that includes several possible alternatives (including series and/or parallel arrangements, involving stream splitting and by-passing) for a set of pre-established matches for the different periods was proposed. The authors also presented a graphical representation aiming to reduce the NLP problem considering changes in the pinch point, identified when the LP problem for each period was solved separately.

In the early 2000's, Aaltola [8] introduced a simultaneous optimization model using mathematical programming to synthesize flexible HEN. In this sense, the author proposed that only one problem, with a mixed integer nonlinear programming (MINLP) formulation, was solved aiming to minimize the TAC simultaneously for all periods of operation. In the synthesis of the flexible HEN, able to operate in all periods, he used a procedure with mean area values and the superstructure proposed by Yee and Grossmann [9]. This superstructure, known in the literature as stage-wise (SWS) superstructure, is, since its proposal, the most used one in the field of synthesis of HENs, flexible or not. It allows streams splitting with isothermal mixing at the end of the stages. By-passes are not supposed to occur. These assumptions mathematically simplify the optimization model, since all constraints are linear. This more simplified model (when compared, for

example, to the superstructure of Floudas and Grossmann [6]) explains the preference for using this superstructure in simultaneous approaches for HENs synthesis.

Some years after the work of Aaltola [8], Verheyen and Zhang [10] modified his model to synthesize a HEN able to operate in multiple periods and whose TAC was calculated using, for each piece of equipment, the maximum heat exchange area among all the periods. These authors also considered the superstructure of Yee and Grossmann [9], but non-isothermal mixing was considered.

MINLP was also used by Chen and Hung [11], in an extension of their previous work [12], which used MINLP for simultaneous synthesis of HENs considering a finite number of operating conditions, followed by flexibility analysis over the full disturbance ranges and integer cuts in order to exclude networks that do not exhibited the necessary flexibility. In the extension of 2007 [11], mass exchange networks with known disturbances in the inlet compositions of the streams were also considered and they substituted the step of flexibility test by applying many simulations with input conditions randomly varied within the possible operating range.

A different superstructure, called IBMS (Interval Based MINLP Superstructure), was used by Isafiade and Fraser [13] in the synthesis of multiperiod HENs. This superstructure, proposed by Isafiade and Fraser [14], uses the supply and target temperatures of either hot or cold set of streams to define its intervals, which avoids the need for nonlinear mixing equations by mixing streams with the same temperature. The proposal of Verheyen and Zhang [10] to use the maximum area for each period was included in the objective function to ensure that the same matching between two streams that exchanged heat in two or more different periods could apply to all periods.

The constraint of using the same match between two streams in each piece of equipment was not adopted by Jiang and Chang [15], since they introduced the so-called

timesharing mechanism for flexible multiperiod HENs. In this scheme, one piece of equipment may be used by different pair of streams in different periods of operation. In their approach a MINLP model is solved separately for each period and heat transfer devices are not constrained to use the same pair of streams in the different periods. Then the flexible multi-period HEN is designed with a procedure that identifies decreasing areas. The approach avoids excessive heat exchange areas during periods with much smaller heat duties and also decreases the complexity of the MINLP model.

Fluctuation in energy prices was considered by Nemet and co-workers [16] in their MINLP formulation, which also considered life expectancy. The objective function considered a trade-off between investment and operating costs. The results showed that it was possible to obtain designs with improved economic performance in terms of the TAC.

More recently, two works [17-18] considered a two-step approach for the synthesis of HENs able to operate in different conditions. In the former, Li et al. [17] used the direction matrix method to provide flexibility and ensure the HEN satisfied critical operating criteria. In the first step, the HEN structure was synthesized with an iterative method using a flexibility test, similar to that of Chen and Hung [12]. In the second step, the area was optimized, taking into consideration its influence on TAC and on the flexibility index. In the latter, Isafiade and co-workers [18] presented a modified version of the Yee and Grossmann [9] superstructure for the synthesis of HENs with multiple periods of operation and with multiple utilities. The isothermal mixing assumption was maintained and no series configuration of split streams in a stage is allowed. The proposed technique consisted of a sequential two-step approach and a set of MINLP models. The authors demonstrate the importance of restricting the utilities to utility stages in the superstructure model.

In 2012, El-Temtamy and Gabr [19] applied the MILP model of Floudas and Grossmann [4] for the design of flexible HENs using random different iterations runs for producing alternative networks. In their discussion they stressed that, due to present world economic situation of rising energy prices, simultaneous approaches for designing flexible HENs might result in flexible HENs that would be optimal for a short time and that returning back to sequential procedures might be an important research decision.

The most recent study that adopts sequential approach in flexible HEN synthesis field is the one of Mian et al. [20]. These authors proposed a sequential approach for the synthesis of HEN with multiple periods of operation and utility systems. The proposed approach adopts a multiperiod utility integration and scheduling model as well as a modified formulation for the MILP multiperiod minimum number of units problem of Floudas and Grossmann [4]. The NLP multiperiod minimum investment network problem proposed by Floudas and Grossmann [6] is solved using a derivative-free hybrid algorithm PGS-COM (Particle Generating Set–Complex), used for black-box nonsmooth problems. In their superstructure parallel and series configurations are considered in the HEN topology.

It is also important to mention the use of non-deterministic optimization methods to solve the problem of flexible HEN synthesis. Ma et al. [21] developed a two steps model for the synthesis of multi-stream heat exchanger networks (MSHEN) for multi-period operation. In the first step, a first version of the multi-period MSHEN is synthesized by the temperature–enthalpy (T – H) diagram. In the second step, the optimal MSHEN obtained in the first stage is improved, using the same structure. Each heat exchanger area is optimized considering the multiperiod operation in order to reduce the MSHEN cost. The total annual cost is calculated by using a genetic/simulated annealing algorithm (GA/SA).

Ahmad et al. [22] presented a case study considering the hydrotreating process in petroleum refineries where the reactor temperature is increased to compensate catalyst deactivation. An optimization approach using simulated annealing for the synthesis of heat exchanger networks for multi-period operation was proposed. Stream splitting, mixing, bypass and multiple matches between pairs of streams were considered in the HEN superstructure, solved by simulated annealing.

Yi et al. [23] presented an optimization method to consider the system reliability analysis for flexible HEN using genetic/simulated annealing algorithms (GA/SA). A connection sequence matrix (CSM) is used to analyze the heat exchanger connections and the independent subsystems in the HEN to achieve the reliability system. The maximum number of heat exchangers in the HEN is used in this analysis. If a HEN did not meet system reliability, some heat exchangers are removed and the system reliability is recalculated. After this process, the devices areas are optimized using then GA/SA. The favorable network configuration, which considers both the most economical cost and system reliability criterion, is located.

Considering all this development in the task of synthesizing multiperiod HEN, in the present paper, it is proposed a sequential approach to the synthesis of multiperiod HENs. In the first step, a LP model is used to identify minimum utilities demand and the pinch point for each period of operation. In the second step, a MILP model that considers the variations in the utilities demand and in the pinch point in each period allows to find stream matches and the minimum number of heat exchangers for all periods at the same time. In the third step a HEN able to operate in all periods is synthesized. It is based on the Non Linear Programming (NLP) model of Floudas and Grossmann [6], which minimizes the total cost of the flexible HEN. However, in the present work, it is proposed a modification in their superstructure and model. Bypasses are added from

upstream one device to downstream another device and two sets and a new parameter are created to reduce the complexity of the mathematical formulation. The NLP model objective is to minimize capital costs, calculated with the required areas of each device in each period. The use of the area of each device in each period is important in order to decrease in the final multiperiod HEN the presence of internal “by-pass” branches in all periods of operation and not only in the period that requires the largest value of area. The superstructure proposed in the present paper and the NLP model formulation are the novelty of the present paper and lead to better results in solving benchmark multiperiod HEN problems, even when the results of a recent paper are considered.

2. DEVELOPED MODEL

Since the approach adopted in this paper is sequential, different optimization models are formulated and solved in sequential steps. Figure 1 illustrates this procedure, along with the presentation of the pertinent nomenclature. Each one of the procedure steps is detailed in the subsequent three sections.

The first step of the procedure has a LP formulation and has as objective the minimization of utilities demand (QS_m and QW_n). An LP problem is formulated and solved for each period separately. At the end of this step, pinch temperatures are known.

In the second step, it is necessary to identify the binary variables $ya_{i,j}$, $yb_{i,j,s}$ and $y_{i,j,s,t}$, which are related to the possible matches, as explained in detail Section 2.2. In this step, only one MILP problem is solved to minimize the number of heat transfer devices of the multiperiod HEN (Z). Also, at the end of this step, the stream matches and the heat loads ($Q_{ij,u,t}$) are known in each device in each period.

Finally, a third step, using an NLP formulation and a new proposed superstructure, is responsible for minimizing the capital cost of the HEN. It provides

automatically the viable topology and heat capacities and temperatures of streams branches. Two sets (Nh and Nc) and a parameter ($Sub_{u,t}$) are proposed to reduce the number of variables and constraints in the NLP problem, as explained in detail Section 2.3.

2.1 First step: LP model

In the first step the minimum utilities demand (QS_m and QW_n) and the pinch point temperature are calculated in each period of operation by a LP model. The objective function to be minimized is the summation of the hot and cold utilities cost, and the constraints are mass and energy balances in the temperature intervals generated by the inlet and outlet temperatures. The reader is referred to Floudas and Grossmann [4] to observe the well-known LP transshipment model for the minimization of utilities costs. At the end of this step, for each period, besides minimal costs of utilities, also pinch temperatures are known. The pinch temperature in each period divides the HEN to be designed into two sub-networks.

2.2 Second step: MILP model

In the second step a MILP model is used to achieve the minimum number of heat exchangers. The model must be solved for all periods at once and for all sub-networks, since it is possible to have different pinch points for the different periods. The MILP solution determines streams matches and the heat amount exchanged in each device in each period. Some remarks are important:

- i) Each heat exchanger must be able to exchange variable heat duty;
- ii) In all periods of operation for each heat exchanger the same hot and cold streams match must be fixed in order to avoid, for example, excessive piping costs;

- iii) If, in a specific period, a pair of streams is necessary in several sub-networks, different heat transfer devices are necessary for each sub-network, so as to avoid large heat exchange areas.

Binary variables $y_{i,j}$ (i is the hot stream or hot utility and j is the cold stream or cold utility) are used to indicate whether a match between two streams exists ($y_{i,j} = 1$) or not ($y_{i,j} = 0$). In this way, depending on the number of process streams and on available utilities, the number of binary variables could be large. To circumvent this disadvantage, Floudas and Grossmann [4] suggested that the pairs of streams must either satisfy only one of the following conditions or not satisfy any of them:

Condition A: the match between the hot stream or utility i with the cold stream or utility j is possible in only one sub-network in each period of operation. The pair (i,j) that satisfies this condition belongs to set Pa ;

Condition B: the match (i,j) is possible in different sub-networks in only one period of operation, named dominant period. In the other periods, this match is possible in only one sub-network. Matches (i,j) that satisfy this condition belong to set Pb .

Variables that satisfy conditions A and B are $ya_{i,j}$ and $yb_{i,j,s}$ respectively, and s is the sub-network index. The summation of the binary variables defined in the dominant period is attributed to the number of heat exchangers for the pair of streams (i,j) in the non-dominant periods when Condition B is satisfied, making it possible one or more matches in the sub-networks in the non-dominant periods. To the pairs that do not satisfy Condition A or B it must be attributed a binary variable $y_{i,j,s,t}$ for each period, in which t stands for the period index.

The indexes, sets, parameters and variables of the MILP model are defined in the Nomenclature. The objective function to be minimized, Equation (1) in the MILP problem, is the number of heat transfer devices (Z) for N periods of operation in K temperature intervals.

$$\min Z = \sum_i \sum_j u_{i,j} \quad (1)$$

The MILP model has as constraints Equations (2) –(11).

Equation (2) represents the constraints for the number of units ($u_{i,j}$) for the pair of streams that satisfy Condition A, situation in which only one device is required for the pair (i,j). When the pair of streams satisfy Condition B, in the dominant period, the pair (i,j) can exchange heat in several sub-networks. So, the variable $u_{i,j}$ is calculated by a summation of binary variables for this period, as presented in Equation (3). Finally, when the pair of streams does not satisfy Condition A or B, individual binary variables $y_{i,j,s,t}$ are assigned to each period and the variable $u_{i,j}$ is calculated by Equation (4).

$$u_{i,j} = ya_{i,j} \quad \forall (i,j) \in Pa \quad (2)$$

$$u_{i,j} = \sum_{s \in IS} yb_{i,j,s} \quad \forall (i,j) \in Pb; t \in d \text{ (i.e., for the dominant period)} \quad (3)$$

$$u_{i,j} \geq \sum_{s \in IS} y_{i,j,s,t} \quad \forall t = 1, \dots, N; (i,j) \notin Pa, Pb \quad (4)$$

Equations (5) and (6) represent the energy balance for the hot stream i and for the cold stream j , respectively, in each temperature interval and in each period of operation. Equation (7) denotes that residual heat from hot streams in the last temperature interval K ($R_{i,K,s,t}$) is zero.

$$R_{i,k,s,t} - R_{i,k-1,s,t} + \sum_{j \in Ca} Q_{i,j,k,s,t} = QHa_{i,k,t} \quad \forall i \in Ha; k \in IT; s \in IS; t = 1, \dots, N \quad (5)$$

$$\sum_{i \in Ha} Q_{i,j,k,s,t} = QCa_{j,k,t} \quad \forall j \in Ca; k \in IT; s \in IS; t = 1, \dots, N \quad (6)$$

$$R_{i,K,s,t} = 0 \quad (7)$$

Logical constraints are used with the purpose of imposing a null heat duty to a match (i,j) whose device does not exist (i.e., whose binary variable is zero). On the other hand, when the binary variable is one, another constraint is required to limit the total heat exchanged for a given pair of streams in a sub-network by an upper bound of heat duty $(U_{i,j,s,t})$. When Condition A holds, Equation (8) is applied. When Condition B holds, Equations (9) and (10) are applied. Finally, when both conditions do not hold, Equation (11) is applied.

$$\sum_{k \in IT} Q_{i,j,k,s,t} - U_{i,j,s,t} \cdot ya_{i,j} \leq 0 \quad \forall (i,j) \in Pa; s \in IS; t = 1, \dots, N \quad (8)$$

$$\sum_{k \in IT} Q_{i,j,k,s,t} - U_{i,j,s,t} \cdot yb_{i,j,s} \leq 0 \quad \forall (i,j) \in Pb; s \in IS; t \in d \quad (9)$$

$$\sum_{k \in IT} Q_{i,j,k,s,t} - U_{i,j,s,t} \cdot u_{i,j} \leq 0 \quad \forall (i,j) \in Pb; s \in IS; t \notin d \quad (10)$$

$$\sum_{k \in IT} Q_{i,j,k,s,t} - U_{i,j,s,t} \cdot y_{i,j,s,t} \leq 0 \quad \forall (i,j) \notin Pa, Pb; s \in IS; t = 1, \dots, N \quad (11)$$

2.3 Third step: NLP model

In the third step, the minimum global cost is obtained by using a NLP model. It provides automatically the viable configuration of a HEN with the minimum cost, minimum number of devices and minimum utilities demand for each period of operation. Heat transfer area for each heat exchanger is also calculated. In the present study, individual superstructures for each stream are proposed, considering all the possible match connections, including parallel and series arrangements and stream splitting. The novelty in the proposition is the inclusion of by-pass streams in the superstructures from upstream one device to downstream another device.

The superstructure developed in this work is depicted in Figure 2 for hot stream $H1$ that can match with two cold streams, $C1$ and $C2$, in the units $U1$ and $U2$, respectively. Figure 2 also brings the nomenclature of variables present in this superstructure, but without indices of variables, for the sake of legibility.

In order to help the reader with these variables and their indices, $Fhsplit5$ can be taken as an example. Its indices are i, j, jj, u, uu and t and this variable in Figure 2 ($Fhsplit5_{H1, C1, C2, U1, U2, t}$) represent the fraction of the flow rate of hot stream $H1$ that, after exchanging heat with cold stream $C1$ in heat exchanger $U1$, is mixed with the other fraction of $H1$ designated to exchange heat with cold stream $C2$ in heat exchanger $U2$, in a specified period t of operation. Analogous multiperiod superstructures can be easily generated for the other hot and cold process streams. In the superstructures for the cold streams, however, the variables are $Fcsplit1_{i,j,u,t}$, $Fcmix1_{i,j,u,t}$, $Tcmix1_{i,j,u,t}$, $Fcsplit2_{i,j,ii,uu,t}$, $Tcsplit2_{i,j,ii,uu,t}$, $Fcsplit3_{i,j,u,t}$, $Tcsplit3_{i,j,u,t}$, $Fcinu_{i,j,u,t}$, $Tcinu_{i,j,u,t}$, $Fcoutu_{i,j,u,t}$, $Tcoutu_{i,j,u,t}$, $Fcmix2_{i,j,u,t}$, $Tcmix2_{i,j,u,t}$, $Fcsplit4_{i,j,u,t}$, $Tcsplit4_{i,j,u,t}$, $Fcsplit5_{i,j,ii,uu,t}$, and $Tcsplit5_{i,j,ii,uu,t}$. The indexes i and ii represent hot streams and hot utilities, j and jj represent cold streams and cold utilities, u and uu represent the heat transfer devices and t represents the period.

The information of each period in the sub-networks can reduce the number of variables and constraints in the NLP, simplifying the problem. In this way, in the present study, two sets, Nh and Nc , are proposed to indicate if hot and cold streams exchange heat in successive sub-networks. Devices that use utilities are not included in these sets. It is also proposed a parameter $Sub_{u,t}$, which indicates the sub-network of the period of operation in which the heat transfer device is present. Data necessary for assigning a value to this parameter are obtained at the end of Step 2 (MILP model).

The indexes, sets, parameters and variables of the NLP model are described in the Nomenclature. The objective function to be minimized, Equation (12) in the NLP problem, is the total cost for N periods of operation.

$$\min TotalCost \quad (12)$$

The NLP model has as constraints Equations (13) –(65).

Mass balances in Splitter 1 and Splitter 2 of the superstructures for hot and cold streams in all periods are represented by Equations (13) - (16).

$$Fh_{i,t} = \sum_j \sum_{u \in SU} Fhsplit1_{i,j,u,t} \quad (13)$$

$$Fc_{j,t} = \sum_i \sum_{u \in SU} Fcsplit1_{i,j,u,t} \quad (14)$$

$$Fhmix1_{i,j,u,t} = Fhsplit3_{i,j,u,t} + Fhinu_{i,j,u,t} + \sum_{jj} \sum_{\substack{uu \in SU \\ \forall uu \neq u}} Fhsplit2_{i,j,jj,u,uu,t} \quad \forall u \in SU \quad (15)$$

$$Fcmix1_{i,j,u,t} = Fcsplit3_{i,j,u,t} + Fcinu_{i,j,u,t} + \sum_{ii} \sum_{\substack{uu \in SU \\ \forall uu \neq u}} Fcsplit2_{i,j,ii,u,uu,t} \quad \forall u \in SU \quad (16)$$

Equations (17) - (22) are the consequences of energy balance in Splitter 2:

$$Thmix1_{i,j,u,t} = Thsplit3_{i,j,u,t} \quad \forall u \in SU \quad (17)$$

$$Thmix1_{i,j,u,t} = Thinu_{i,j,u,t} \quad \forall u \in SU \quad (18)$$

$$Thmix1_{i,j,u,t} = Thsplit2_{i,j,jj,u,uu,t} \quad \forall u \in SU; uu \in SU; u \neq uu \quad (19)$$

$$Tcmix1_{i,j,u,t} = Tcsplit3_{i,j,u,t} \quad \forall u \in SU \quad (20)$$

$$Tcmix1_{i,j,u,t} = Tcinu_{i,j,u,t} \quad \forall u \in SU \quad (21)$$

$$Tcmix1_{i,j,u,t} = Tcsplit2_{i,j,ii,u,uu,t} \quad \forall u \in SU; uu \in SU; u \neq uu \quad (22)$$

Mass balances in Splitter 3 are represented by Equations (23) and (24), while energy balance in this splitter imposes Equations (25) - (28).

$$Fhmix2_{i,j,u,t} = Fhsplit4_{i,j,u,t} + \sum_{jj} \sum_{\substack{uu \in SU \\ \forall uu \neq u}} Fhsplit5_{i,j,jj,u,uu,t} \quad \forall u \in SU \quad (23)$$

$$F_{cmix2_{i,j,u,t}} = F_{csplit4_{i,j,u,t}} + \sum_{ii} \sum_{\substack{uu \in SU \\ \forall uu \neq u}} F_{csplit5_{i,j,ii,u,uu,t}} \quad \forall u \in SU \quad (24)$$

$$T_{hmix2_{i,j,u,t}} = T_{hsplit4_{i,j,u,t}} \quad \forall u \in SU \quad (25)$$

$$T_{hmix2_{i,j,u,t}} = T_{hsplit5_{i,j,jj,u,uu,t}} \quad \forall u \in SU; uu \in SU; u \neq uu \quad (26)$$

$$T_{cmix2_{i,j,u,t}} = T_{csplit4_{i,j,u,t}} \quad \forall u \in SU \quad (27)$$

$$T_{cmix2_{i,j,u,t}} = T_{csplit5_{i,j,ii,u,uu,t}} \quad \forall u \in SU; uu \in SU; u \neq uu \quad (28)$$

Equations (29) and (30) are the mass balances in Mixer 1, while energy balance in this mixer leads to Equations (31) and (32).

$$F_{hsplit1_{i,j,u,t}} + \sum_{jj} \sum_{\substack{uu \in SU \\ \forall uu \neq u}} F_{hsplit5_{i,j,j,uu,u,t}} = F_{hmix1_{i,j,u,t}} \quad \forall u \in SU \quad (29)$$

$$F_{csplit1_{i,j,u,t}} + \sum_{ii} \sum_{\substack{uu \in SU \\ \forall uu \neq u}} F_{csplit5_{ii,j,i,uu,u,t}} = F_{cmix1_{i,j,u,t}} \quad \forall u \in SU \quad (30)$$

$$\begin{aligned} F_{hsplit1_{i,j,u,t}} \cdot T_{hin_{i,t}} + \sum_{jj} \sum_{\substack{uu \in SU \\ \forall uu \neq u}} (F_{hsplit5_{i,j,j,uu,u,t}} \cdot T_{hsplit5_{i,j,j,uu,u,t}}) \\ = F_{hmix1_{i,j,u,t}} \cdot T_{hmix1_{i,j,u,t}} \quad \forall u \in SU \end{aligned} \quad (31)$$

$$\begin{aligned} F_{csplit1_{i,j,u,t}} \cdot T_{cin_{j,t}} + \sum_{ii} \sum_{\substack{uu \in SU \\ \forall uu \neq u}} (F_{csplit5_{ii,j,i,uu,u,t}} \cdot T_{csplit5_{ii,j,i,uu,u,t}}) \\ = F_{cmix1_{i,j,u,t}} \cdot T_{cmix1_{i,j,u,t}} \quad \forall u \in SU \end{aligned} \quad (32)$$

In Mixer 2, the mass balances are given by Equations (33) and (34), while Equations (35) and (36) are the corresponding energy balances.

$$F_{houtu_{i,j,u,t}} + F_{hsplit3_{i,j,u,t}} + \sum_{jj} \sum_{\substack{uu \in SU \\ \forall uu \neq u}} F_{hsplit2_{i,j,j,uu,u,t}} = F_{hmix2_{i,j,u,t}} \quad \forall u \in SU \quad (33)$$

$$F_{coutu_{i,j,u,t}} + F_{csplit3_{i,j,u,t}} + \sum_{ii} \sum_{\substack{uu \in SU \\ \forall uu \neq u}} F_{csplit2_{ii,j,i,uu,u,t}} = F_{cmix2_{i,j,u,t}} \quad \forall u \in SU \quad (34)$$

$$\begin{aligned}
 & Fhout_{i,j,u,t} \cdot Thout_{i,j,u,t} + Fhsplit3_{i,j,u,t} \cdot Thsplit3_{i,j,u,t} \\
 & + \sum_{jj} \sum_{\substack{uu \in SU \\ \forall uu \neq u}} (Fhsplit2_{i,j,j,uu,u,t} \cdot Thsplit2_{i,j,j,uu,u,t})
 \end{aligned} \tag{35}$$

$$= Fhmix2_{i,j,u,t} \cdot Thmix2_{i,j,u,t} \quad \forall u \in SU$$

$$\begin{aligned}
 & Fcout_{i,j,u,t} \cdot Tcout_{i,j,u,t} + Fcsplit3_{i,j,u,t} \cdot Tcsplit3_{i,j,u,t} \\
 & + \sum_{ii} \sum_{\substack{uu \in SU \\ \forall uu \neq u}} (Fcsplit2_{ii,j,i,uu,u,t} \cdot Tcsplit2_{ii,j,i,uu,u,t})
 \end{aligned} \tag{36}$$

$$= Fcmix2_{i,j,u,t} \cdot Tcmix2_{i,j,u,t} \quad \forall u \in SU$$

In an analogous way, for Mixer 3, mass and energy balances are written in Equations (37) – (40).

$$\sum_j \sum_{u \in SU} Fhsplit4_{i,j,u,t} = Fh_{i,t} \tag{37}$$

$$\sum_i \sum_{u \in SU} Fcsplit4_{i,j,u,t} = Fc_{j,t} \tag{38}$$

$$\sum_j \sum_{u \in SU} (Fhsplit4_{i,j,u,t} \cdot Thsplit4_{i,j,u,t}) = Fh_{i,t} \cdot Thout_{i,t} \tag{39}$$

$$\sum_i \sum_{u \in SU} (Fcsplit4_{i,j,u,t} \cdot Tcsplit4_{i,j,u,t}) = Fc_{j,t} \cdot Tcout_{j,t} \tag{40}$$

Equations (41) and (42) ensure that streams that exchange heat in different devices located in different sub-networks have, in the upper sub-network, outlet temperature values not lower than those in the lower sub-network.

$$Thout_{i,j,u,t} \geq Thout_{i,j,j,uu,t} \quad \forall u \in SU; uu \in SU; i \in Nh; Sub_{u,t} < Sub_{uu,t} \tag{41}$$

$$Tcout_{i,j,u,t} \geq Tcout_{ii,j,uu,t} \quad \forall u \in SU; uu \in SU; j \in Nc; Sub_{u,t} < Sub_{uu,t} \tag{42}$$

Equations (43) and (44) are specific to problems with only one pinch point and are responsible for putting in series all heat transfer devices that are in successive sub-networks. For problems that have more than one pinch points, others constraints should be added manually.

$$\sum_{\substack{uu \in SU \\ \forall Sub_{uu,t}=2}} \sum_{u \in SU} \sum_{\substack{jj \notin n \\ j}} \sum_j Fhsplit5_{i,j,jj,u,uu,t} \leq \sum_{\substack{uu \in SU \\ \forall Sub_{uu,t}=2}} \sum_{\substack{jj \notin n}} Fhmix1_{i,jj,uu,t} \quad \forall i \notin m \quad (43)$$

$$\sum_{\substack{uu \in SU \\ \forall Sub_{uu,t}=1}} \sum_{u \in SU} \sum_{\substack{ii \notin m \\ i}} \sum_i Fcsplit5_{i,j,ii,u,uu,t} \leq \sum_{\substack{uu \in SU \\ \forall Sub_{uu,t}=1}} \sum_{\substack{ii \notin m}} Fcmix1_{ii,j,uu,t} \quad \forall j \notin n \quad (44)$$

The temperature differences in the hot and in the cold ends of the heat exchanger must be greater than or equal to the minimal approach temperature. It is assured by Equations (45) and (46).

$$d1_{u,t} \geq \Delta T_{min} \quad (45)$$

$$d2_{u,t} \geq \Delta T_{min} \quad (46)$$

Equations (47) and (48) are the mass balances in each heat transfer device. Energy balance for hot stream and cold streams in each device and in each period of operation are given, respectively, by Equations (49) and (50). The heat duty in the device u in the period t of operation ($Qu_{u,t}$) is identical to $Qij_{u,t}$, the heat duty for the pair (i, j) of the MILP problem solution for the pairs of streams belonging to the sets Pm in the dominant period and Pl (Equations (51) and (52)). The pairs of streams that belong to the set Pm in the non-dominant periods must satisfy the constraint in Equation (53), which determines that the sum of all heat duties calculates for the pair (i, j) in the different devices must be equal to the heat duty calculated in the MILP model.

$$Fhinu_{i,j,u,t} = Fhoutu_{i,j,u,t} \quad \forall u \in SU \quad (47)$$

$$Fcinu_{i,j,u,t} = Fcoutu_{i,j,u,t} \quad \forall u \in SU \quad (48)$$

$$Qu_{u,t} = Fhinu_{i,j,u,t} \cdot (Thinu_{i,j,u,t} - Thoutu_{i,j,u,t}) \quad \forall u \in SU \quad (49)$$

$$Qu_{u,t} = Fcinu_{i,j,u,t} \cdot (Tcoutu_{i,j,u,t} - Tcinu_{i,j,u,t}) \quad \forall u \in SU \quad (50)$$

$$Qu_{u,t} = Qij_{u,t} \quad \forall u \in SU; (i, j) \in Pl \quad (51)$$

$$Qu_{u,t} = Qij_{u,t} \quad \forall u \in SU; (i, j) \in Pm; t \in d \quad (52)$$

$$\sum_{u \in SU} Qu_{u,t} = Qij_{u,t} \quad \forall (i,j) \in Pm; t \notin d \quad (53)$$

Equations (54) – (61) are necessary in order to achieve series heat transfer devices in successive sub-networks for those pairs of streams that exchange heat in different devices.

$$Fhsplit5_{i,j,j,uu,u,t} = 0 \quad \forall u \in SU; uu \in SU; i \in Nh; Sub_{u,t} \leq Sub_{uu,t} \quad (54)$$

$$Fcsplit5_{i,j,ii,u,uu,t} = 0 \quad \forall u \in SU; uu \in SU; j \in Nc; Sub_{u,t} \leq Sub_{uu,t} \quad (55)$$

$$Fhsplit5_{i,j,j,uu,u,t} = 0 \quad \forall u \in SU; uu \in SU; Sub_{u,t} = Sub_{uu,t} \quad (56)$$

$$Fcsplit5_{i,j,ii,u,uu,t} = 0 \quad \forall u \in SU; uu \in SU; Sub_{u,t} = Sub_{uu,t} \quad (57)$$

$$Fhsplit2_{i,j,j,uu,u,t} = 0 \quad \forall u \in SU; uu \in SU; i \in Nh; Sub_{u,t} \leq Sub_{uu,t} \quad (58)$$

$$Fcsplit2_{i,j,ii,u,uu,t} = 0 \quad \forall u \in SU; uu \in SU; j \in Nc; Sub_{u,t} \leq Sub_{uu,t} \quad (59)$$

$$Fhsplit2_{i,j,j,uu,u,t} = 0 \quad \forall u \in SU; uu \in SU; Sub_{u,t} = Sub_{uu,t} \quad (60)$$

$$Fcsplit2_{i,j,ii,u,uu,t} = 0 \quad \forall u \in SU; uu \in SU; Sub_{u,t} = Sub_{uu,t} \quad (61)$$

Heat exchanger hot and cold ends temperature differences are calculated by Equations (62) and (63), respectively.

$$d1_{u,t} = Thinu_{i,j,u,t} - Tcoutu_{i,j,u,t} \quad \forall u \in SU \quad (62)$$

$$d2_{u,t} = Thoutu_{i,j,u,t} - Tcinu_{i,j,u,t} \quad \forall u \in SU \quad (63)$$

The heat transfer area of device u in period t of operation is calculated by Equation (64). Capital cost is given by Equation (65), where a , b and c are constant cost coefficients.

$$Qu_{u,t} = Co_u \cdot Area_{u,t} \cdot LMTD_{u,t} \quad (64)$$

$$TotalCost = \sum_u \sum_t (a + b \cdot Area_{u,t}^c) \quad (65)$$

Finally, with the largest heat transfer area among all calculated areas for the same device in all periods of operation ($AreaM_u$), the cost of that heat exchanger can be calculated:

$$TotalCost1 = \sum_u (a + b \cdot AreaM_u^c) \quad (66)$$

It is important to stress that the objective function is calculated with the required areas for each device in each period. It is important to use this variable (area for each device in each period) in the objective function and not the largest heat transfer area among all calculated areas for the same device in all periods of operation in order to decrease, in the final multiperiod HEN, the presence of internal “by-pass” branches (*Fhsplit2* and *Fhsplit5* of Figure. 2) in all periods of operation and not only in the period that requires the largest value of area. This is due to the fact that the greater the number of internal “by-pass” streams in a superstructure, the lower the logarithmic mean temperature difference, which leads to larger areas, and, consequently, to higher capital costs.

3. CASE STUDIES

Two examples from the literature were used to test the model applicability. Models were solved in GAMS, in the version 24.7.1. in an Intel Core 5, 2.60 GHz.

3.1 Example 1

This example was originally presented by Floudas and Grossmann [6] and it was also used by Isafiade and Fraser [13], Isafiade et al. [18] and Mian et al. [20]. The problem has two hot and two cold streams, one hot utility (*HU*, steam) and one cold utility (*CU*, cold water). Three periods of operation were considered. Heat capacities (*F*) and inlet (*T_{in}*) and outlet (*T_{out}*) temperatures can vary from one period to another and are presented in Table 1. The steam temperature is supposed to be 300 °C. Cold water inlet and outlet temperatures are 30 and 50 °C, respectively. 10 °C is used as the minimum approach temperature, as proposed by Floudas and Grossmann [6].

The LP model was solved for each period of operation with solver CPLEX 12.6, requiring less than 1 second. Hot and cold utilities demands QS_m and QW_n as well as the pinch point are presented in Table 2. It can be observed that the utilities demand vary from one period to another. The same occurs with the pinch point temperatures. Period 2 has no sub-networks, since it comprises a threshold problem.

With data obtained by the LP model and with information of sub-networks presented in Figure 3, based on Floudas and Grossmann [4], it is possible to identify pairs of streams that satisfy Conditions A and B. Pairs H1-C1, H1-C2, H1-CU, H2-C1, H2-CU, HU-C1 and HU-C2 satisfy Condition A, because they can exchange heat in only one sub-network in each period of operation. Pair H2-C2 satisfies Condition B, because these streams can exchange heat in both sub-networks of period 1 and in only one sub-network in period 2 and in period 3.

Considering these results as inlet data for the MILP model, it is possible to identify 7 binary variables $ya_{i,j}$ and two binary variables $yb_{i,j,s}$, one for each sub-network. The MILP model is then formulated without using the binary variable $y_{i,j,s,t}$. Instead, only variables $ya_{i,j}$ and $yb_{i,j,s}$ are used because every possible match satisfy one of the conditions. Finally, the model has 9 binary variables and was solved with CPLEX 12.6, requiring less than 1 second.

The best network topology has 7 heat transfer devices. This number of devices was also found by Floudas and Grossmann [6] but in their work different heat duties are assigned to each device. Matches of this work and corresponding duties for each period are presented in Table 3.

With the MILP results it is possible to identify that the parameter $Sub_{u,t}$ value is 1 for all heat transfer devices in period 2 because there are no sub-networks. In periods 1 and 3 its value is 1 for device $U1$ and 2 for devices $U3$, $U4$, $U5$, $U6$ and $U7$. For device

$U2$, its value is 1 for period 1 and is 2 for period 3. It can also be noted that the cold utility must be renamed to $CU1$ and $CU2$ because it is used in devices $U6$ and $U7$.

Matches are divided into two sets. The set Pl is composed by matches $H1-C1$, $H1-C2$, $H1-CU1$, $H2-CU2$ and $HU-C2$. The set Pm is composed by match $H2-C2$ and period 1 is the dominant one. As proposed in the present work, it is possible to generate the sets Nh and Nc to aid in simplifying superstructures. $H2-U2-U5-T1$ composes Nh , while $C2-U2-U4-T1$ and $C2-U2-U5-T1$ compose Nc .

In the third step, when using the NLP model, the minimum approach temperature is relaxed to $0.1\text{ }^{\circ}\text{C}$, based on Floudas and Grossmann [6]. The NLP model was solved with the solver CONOPT3, requiring less than 1 second. Table 4 shows individual areas of the heat transfer devices, as well the global heat transfer coefficients and cost data used in the model (values presented by Floudas and Grossmann [6]).

Figures 4 and 5 show the best network topology and information on heat capacities and streams temperature in each point of the network in each period. This HEN is viable in all operation periods. It can be noted that the optimization procedure determined that $C2$ and $H1$ should be split. Two coolers are not used in period 2 and there are by-passes in streams $C2$, $H1$ and $H2$.

The HEN proposed by the methodology developed in the present work has the same utilities costs as Floudas and Grossmann [6], but presents lower capital cost, as shown in Table 5. Furthermore, there are less by-pass structures than the result presented by Floudas and Grossmann [6], which decreases costs for the HEN implementation. In Table 5, results of this study are also compared to those of Isafiade and Fraser [13], Isafiade *et al.* [18] and Mian *et al.* [20]. In both papers, Isafiade and Fraser [13] and Isafiade *et al.* [18], authors gave priority to minimize capital cost but the utilities cost was extremely increased.

Table 6 shows a comparison among the annualized costs, considering 8600 hours of operation in one year and equal duration for the periods. It can be seen that the utilities cost influences highly the final cost. It is important to note that in the work of Mian et al. [20] it was considered 6000 hours of operation in one year, in three equal periods of 2000 hours, with an annualizing factor of 0.27. In order to compare the results of the present study with the work of Mian et al. [20], their results were converted to 8600 hours of operation per year and an annualizing factor equal to 0.2 was used. This comparison is valid because the periods have the same duration and because the calculation of the utilities cost is provided in the first LP step.

It is possible to conclude that the optimal values found by the authors Floudas and Grossmann [6], Isafiade and Fraser [13], Isafiade et al. [18] and Mian et al. [20] are local optimum. In the paper of Isafiade et al. [18], the HEN presented did not exhibit any heat integration, since there was no heat exchange between the process streams. Only heaters and coolers were used, so capital costs were low, as expected, while utility costs were large. Also, the TAC values were incorrectly presented in $\$/h$, instead of $\$/year$ (TAC stands for total annualized cost). This could mean that capital cost was added (without transforming it to $\$/h$) to the utility costs on an hourly basis, which would explain the value of 125,371 $\$/h$ presented in their work.

The sequential procedure using the superstructure proposed in the present work enabled finding a better result for the final cost.

3.2 - Example 2

This problem was adapted from Floudas and Grossmann [25], and it was used by Isafiade and Fraser [13] and also solved by Chen and Hung [12]. There are two hot and two cold streams, one hot and one cold utility, operating in four different periods. Temperatures and flow rates can vary. Table 7 presents data of Example 2.

The LP model was solved for each period of operation with a minimum temperature approach of 20 K. The solver CPLEX 12.6 was used and the problem was solved in less than 1 second. Table 8 presents the utilities demand and the pinch point (that exists only for period 3). Remaining periods need only cold utility.

Using these results, with an analogous analysis as that made for the results of LP model in Example 1, the MILP model for Example 2 is formulated using only the binary variable $ya_{i,j}$ since matches $H1-C1$, $H1-C2$, $H1-CU$, $H2-C1$, $H2-C2$, $H2-CU$, $HU-C1$ and $HU-C2$ satisfy Condition A. So, 8 binary variables are necessary. The solver CPLEX 12.6 solved the problem in less than 1 second.

For the HEN topology found by the MILP model, only six heat transfer devices were necessary because $ya_{i,j}$ variables for matches $HU-C2$ and $H2-CU$ were equal to zero. Table 9 shows this configuration and corresponding heat duties (kW) for each period.

Parameter $Sub_{u,t}$ assumes value 1 in all heat transfer devices of the period with nominal conditions, in periods 1 and 2 and in period 3 for devices $U1$, $U2$, $U3$, $U4$ and $U5$. It assumes value 2 in period 3 for device $U6$. All stream matches belong to the set Pl .

CONOPT3 required less than 1 second to solve the NLP model, with minimum approach temperature of 10 K and with global heat transfer coefficients and cost data presented in Table 10. This table also brings the individual areas of the heat transfer devices.

Figure 6 presents the HEN topology, viable in all operation periods. Figure 7 shows information on heat capacities and streams temperature in each point of the network in each period. Table 11 presents capital and utilities costs found in this study. All periods have the same duration and it was considered 8600 hours per year.

Table 12 presents a comparison among the annualized costs of this work and those of Floudas and Grossmann [25], Chen and Hung [12] and Isafiade and Fraser [13].

Figure 8 presents the HEN configuration of Isafiade and Fraser [13]. It is possible to verify that device U5 in this HEN has very small area and heat duty, characterizing a micro heat exchanger. In practice, such a small device does not exist in industrial real processes. Authors should consider the alternative of removing this heat exchanger from the HEN and recalculating the total cost. Although the optimal HEN obtained in the present study has a higher cost than those of Isafiade and Fraser [13], it is feasible in practice. It does not occur with the Isafiade and Fraser [13] network, which is a simple mathematical calculation without industrial applicability. Considering no micro heat exchangers are present, the HEN synthesized using the methodology proposed in the present paper is better than the final HEN of Isafiade and Fraser [13] for process control and operability purposes, although it presents a higher global annualized cost.

4. CONCLUSIONS

The synthesis of multiperiod HEN can be formulated as an optimization problem. In the present work an approach was proposed to solve the problem, in three sequential steps, represented by LP, MILP and NLP models, aiming to achieve the minimum global cost with the minimal number of heat transfer devices and utilities demand. In sequential approaches, the solution found for a problem serves as input to the next problem. The major advantage is the fact that simpler optimization problems are solved sequentially, when compared to simultaneous approaches, which solves only one optimization problem for the HEN synthesis. Individual superstructures for each process stream, based on the work of Floudas and Grossmann [6], were proposed, considering all the possible match connections, including parallel and series arrangements and stream splitting. The

novelty in the superstructure is the inclusion of by-pass streams, from upstream one device to downstream another device. Furthermore, information on the sub-networks of each period is used to reduce the complexity of the NLP model in the third step of the sequential methodology, simplifying the problem. So, two sets, Nh and Nc , were proposed to indicate if hot and cold process streams exchange heat in successive sub-networks. It was also proposed the parameter Sub that indicates the sub-network of the period of operation in which the heat transfer device is present. The NLP model evaluates the objective function with the required areas of each device in each period.

Two case studies were used to test the applicability of the developed methodology and results were better when compared to findings published previously in the literature. Results show, in the first case study, a better minimum annualized cost, including a comparison with a recent paper and, in the second one, a more feasible HEN topology, considering industrial applications, although with a little higher total annual cost.

5. NOMENCLATURE

5.1 – MILP model

5.1.1 Indexes

i	hot process stream or hot utility
j	cold process stream or cold utility
k	temperature interval
s	subnetwork
t	period of operation

5.1.2 Sets

Ca	set of cold streams and cold utilities that can accept heat in a specified temperature interval of a period
d	dominant period of a pair of streams
Ha	set of hot streams and hot utilities that can transfer heat in a specified temperature interval, or in a superior temperature interval, of a period
IS	sub-networks in the period of operation
IT	set of temperature intervals belonging to a specific sub-network
Pa	set containing pairs (i, j) of streams that satisfy Condition A
Pb	set containing pairs (i, j) of streams that satisfy Condition B

5.1.3 Parameters

K	number of temperature intervals
N	number of periods
$QCa_{j,k,t}$	heat duty between cold stream j and hot utilities in the k^{th} temperature interval in period t (defined by the LP problem solution) [kW]
$QHa_{i,k,t}$	heat duty between hot stream i and cold utilities in the k^{th} temperature interval in period t (defined by the LP problem solution) [kW]
$U_{i,j,s,t}$	upper bound of heat duty for pair (i, j) of streams in sub-network s in period t [kW]

5.1.4 Binary variables

ya_{ij}	indicates the existence of heat exchange between pair (i, j) of streams that satisfy Condition A
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- $y_{b_{i,j},s}$ indicates the existence of heat exchange, in sub-network s , between pair (i, j) of streams that satisfy Condition B
- $y_{i,j,s,t}$ indicates the existence of heat exchange, in sub-network s in period t , between pair (i, j) of streams that satisfy neither Condition A nor Condition B

5.1.5 Integer positive variables

- $u_{i,j}$ number of heat transfer devices for pair (i, j) of streams
- Z number of heat transfer devices for N periods of operation in K temperature intervals

5.1.6 Real positive variables

- $Q_{i,j,k,s,t}$ heat duty of pair (i, j) of streams in the k^{th} temperature interval in sub-network s in period t [kW]
- $R_{i,k,s,t}$ residual heat from hot stream i in the k^{th} temperature interval in sub-network s in period t [kW]

5.2 – NLP model

5.2.1 Indexes

- i hot process stream or hot utility
- ii hot process stream or hot utility
- j cold process stream or cold utility
- jj cold process stream or cold utility
- t period of operation
- u heat transfer device
- uu heat transfer device

5.2.2 Sets

m	set of hot utilities
n	set of cold utilities
N_c	set that indicates if cold streams exchange heat in successive sub-networks
N_h	set that indicates if hot streams exchange heat in successive sub-networks
Pl	set formed by the pairs of streams that have only one heat transfer device in each sub-network in all periods
Pm	set formed by the pairs of streams that have more than one heat transfer device in a sub-network in at least one period
SU	set that contains information on the pair (i, j) of streams that exchange heat in each heat transfer device

5.2.3 Parameters

a, b and c	coefficients in the cost equation
Co_u	global heat transfer coefficient of heat exchanger u [kW/(m ² K)]
$FC_{j,t}$	heat capacity of cold stream j in period t of operation [kW/K]
$Fh_{i,t}$	heat capacity of hot stream i in period t of operation [kW/K]
$Qij_{u,t}$	heat duty of pair (i, j) of streams in heat transfer device u in period t of operation (defined by the MILP problem solution) [kW]
$Sub_{u,t}$	sub-network of period t of operation in which the heat exchanger u is present
$Tcin_{j,t}$	inlet temperature of cold stream j in period t of operation [K or °C]

$T_{cout,j,t}$	outlet temperature of cold stream j in period t of operation [K or °C]
$Thin_{i,t}$	inlet temperature of hot stream i in period t of operation [K or °C]
$Thout_{i,t}$	outlet temperature of hot stream i in period t of operation [K or °C]
Δmin	minimal approach temperature [K or °C]

5.2.4 Positive variables

$AreaM_u$	maximum value for the heat exchanger area among the periods [m ²]
$Area_{u,t}$	heat transfer area of device u in period t of operation [m ²]
$d1_{u,t}$	temperature difference in the hot end of heat exchanger u in period t of operation [K or °C]
$d2_{u,t}$	temperature difference in the cold end of heat exchanger u in period t of operation [K or °C]
$LMTD_{u,t}$	logarithmic mean temperature difference of heat exchanger u in period t of operation, calculated with Chen approximation (Chen [24]) [K or °C]
$Fcinu_{i,j,u,t}$	heat capacity of cold stream j branch that goes from Splitter 2 of its superstructure until heat transfer device u , in which it exchanges heat with hot stream i in period t of operation [kW/K]
$Fcmix1_{i,j,u,t}$	heat capacity of cold stream j branch that goes from Mixer 1 of its superstructure until Splitter 2 upstream heat transfer device u , in which cold stream j exchanges heat with hot stream i in period t of operation [kW/K]
$Fcmix2_{i,j,u,t}$	heat capacity of cold stream j branch that goes from Mixer 2 of its superstructure until Splitter 3 downstream heat transfer device u , in

which cold stream j exchanges heat with hot stream i in period t of operation [kW/K]

$F_{coutu_{i,j,u,t}}$ heat capacity of cold stream j branch that goes from heat transfer device u , in which it exchanges heat with hot stream i , until Mixer 2 of its superstructure in period t of operation [kW/K]

$F_{csplit1_{i,j,u,t}}$ heat capacity of cold stream j branch that goes from Splitter 1 of its superstructure until Mixer 1 upstream heat transfer device u , in which cold stream j exchanges heat with hot stream i in period t of operation [kW/K]

$F_{csplit2_{i,j,ii,u,uu,t}}$ heat capacity of cold stream j branch of its superstructure that goes from Splitter 2 upstream heat transfer device u , in which cold stream j exchanges heat with hot stream i , until Mixer 2 downstream heat transfer device uu , in which cold stream j exchanges heat with hot stream ii in period t of operation [kW/K]

$F_{csplit3_{i,j,u,t}}$ heat capacity of cold stream j branch that by-passes heat transfer device u in which cold stream j exchanges heat with hot stream i in period t of operation [kW/K]

$F_{csplit4_{i,j,u,t}}$ heat capacity of cold stream j branch that goes from Splitter 3 downstream heat transfer device u , in which cold stream j exchanges heat with hot stream i in period t of operation, until Mixer 3, located at the outlet of its superstructure [kW/K]

$F_{csplit5_{i,j,ii,u,uu,t}}$ heat capacity of cold stream j branch of its superstructure that goes from Splitter 3 downstream heat transfer device u , in which cold stream j exchanges heat with hot stream i , until Mixer 1 upstream

- heat transfer device uu , in which cold stream j exchanges heat with hot stream ii in period t of operation [kW/K]
- $Fhinu_{i,j,u,t}$ heat capacity of hot stream i branch that goes from Splitter 2 of its superstructure until heat transfer device u , in which it exchanges heat with cold stream j in period t of operation [kW/K]
- $Fhmix1_{i,j,u,t}$ heat capacity of hot stream i branch that goes from Mixer 1 of its superstructure until Splitter 2 upstream heat transfer device u , in which hot stream i exchanges heat with cold stream j in period t of operation [kW/K]
- $Fhmix2_{i,j,u,t}$ heat capacity of hot stream i branch that goes from Mixer 2 of its superstructure until Splitter 3 downstream heat transfer device u , in which hot stream i exchanges heat with cold stream j in period t of operation [kW/K]
- $Fhoutu_{i,j,u,t}$ heat capacity of hot stream i branch that goes from heat transfer device u , in which it exchanges heat with cold stream j , until Mixer 2 of its superstructure in period t of operation [kW/K]
- $Fhsplit1_{i,j,u,t}$ heat capacity of hot stream i branch that goes from Splitter 1 of its superstructure until Mixer 1 upstream heat transfer device u , in which hot stream i exchanges heat with cold stream j in period t of operation [kW/K]
- $Fhsplit2_{i,j,jj,u,uu,t}$ heat capacity of hot stream i branch of its superstructure that goes from Splitter 2 upstream heat transfer device u , in which hot stream i exchanges heat with cold stream j , until Mixer 2 downstream heat transfer device uu , in which hot stream i exchanges heat with cold stream jj in period t of operation [kW/K]

- $Fhsplit3_{i,j,u,t}$ heat capacity of hot stream i branch that by-passes heat transfer device u in which hot stream i exchanges heat with cold stream j in period t of operation [kW/K]
- $Fhsplit4_{i,j,u,t}$ heat capacity of hot stream i branch that goes from Splitter 3 downstream heat transfer device u , in which hot stream i exchanges heat with cold stream j in period t of operation, until Mixer 3, located at the outlet of its superstructure [kW/K]
- $Fhsplit5_{i,j,jj,u,uu,t}$ heat capacity of hot stream i branch of its superstructure that goes from Splitter 3 downstream heat transfer device u , in which hot stream i exchanges heat with cold stream j , until Mixer 1 upstream heat transfer device uu , in which hot stream i exchanges heat with cold stream jj in period t of operation [kW/K]
- $Tcinu_{i,j,u,t}$ temperature of cold stream j branch that goes from Splitter 2 of its superstructure until heat transfer device u , in which it exchanges heat with hot stream i in period t of operation [K or °C]
- $Tcmix1_{i,j,u,t}$ temperature of cold stream j branch that goes from Mixer 1 of its superstructure until Splitter 2 upstream heat transfer device u , in which cold stream j exchanges heat with hot stream i in period t of operation [K or °C]
- $Tcmix2_{i,j,u,t}$ temperature of cold stream j branch that goes from Mixer 2 of its superstructure until Splitter 3 downstream heat transfer device u , in which cold stream j exchanges heat with hot stream i in period t of operation [K or °C]

- $T_{coutu_{i,j,u,t}}$ temperature of cold stream j branch that goes from heat transfer device u , in which it exchanges heat with hot stream i , until Mixer 2 of its superstructure in period t of operation [K or °C]
- $T_{csplit2_{i,j,ii,u,uu,t}}$ temperature of cold stream j branch of its superstructure that goes from Splitter 2 upstream heat transfer device u , in which cold stream j exchanges heat with hot stream i , until Mixer 2 downstream heat transfer device uu , in which cold stream j exchanges heat with hot stream ii in period t of operation [K or °C]
- $T_{csplit3_{i,j,u,t}}$ temperature of cold stream j branch that by-passes heat transfer device u in which cold stream j exchanges heat with hot stream i in period t of operation [K or °C]
- $T_{csplit4_{i,j,u,t}}$ temperature of cold stream j branch that goes from Splitter 3 downstream heat transfer device u , in which cold stream j exchanges heat with hot stream i in period t of operation, until Mixer 3, located at the outlet of its superstructure [K or °C]
- $T_{csplit5_{i,j,ii,u,uu,t}}$ temperature of cold stream j branch of its superstructure that goes from Splitter 3 downstream heat transfer device u , in which cold stream j exchanges heat with hot stream i , until Mixer 1 upstream heat transfer device uu , in which cold stream j exchanges heat with hot stream ii in period t of operation [K or °C]
- $Thinu_{i,j,u,t}$ temperature of hot stream i branch that goes from Splitter 2 of its superstructure until heat transfer device u , in which it exchanges heat with cold stream j in period t of operation [K or °C]
- $Thmix1_{i,j,u,t}$ temperature of hot stream i branch that goes from Mixer 1 of its superstructure until Splitter 2 upstream heat transfer device u , in

which hot stream i exchanges heat with cold stream j in period t of operation [K or °C]

$Th_{mix2_{i,j,u,t}}$ temperature of hot stream i branch that goes from Mixer 2 of its superstructure until Splitter 3 downstream heat transfer device u , in which hot stream i exchanges heat with cold stream j in period t of operation [K or °C]

$Th_{outu_{i,j,u,t}}$ temperature of hot stream i branch that goes from heat transfer device u , in which it exchanges heat with cold stream j , until Mixer 2 of its superstructure in period t of operation [K or °C]

$Th_{split2_{i,j,jj,u,uu,t}}$ temperature of hot stream i branch of its superstructure that goes from Splitter 2 upstream heat transfer device u , in which hot stream i exchanges heat with cold stream j , until Mixer 2 downstream heat transfer device uu , in which hot stream i exchanges heat with cold stream jj in period t of operation [K or °C]

$Th_{split3_{i,j,u,t}}$ temperature of hot stream i branch that by-passes heat transfer device u in which hot stream i exchanges heat with cold stream j in period t of operation [K or °C]

$Th_{split4_{i,j,u,t}}$ temperature of hot stream i branch that goes from Splitter 3 downstream heat transfer device u , in which hot stream i exchanges heat with cold stream j in period t of operation, until Mixer 3, located at the outlet of its superstructure [K or °C]

$Th_{split5_{i,j,jj,u,uu,t}}$ temperature of hot stream i branch of its superstructure that goes from Splitter 3 downstream heat transfer device u , in which hot stream i exchanges heat with cold stream j , until Mixer 1 upstream

	heat transfer device uu , in which hot stream i exchanges heat with cold stream jj in period t of operation [K or °C]
$Qu_{u,t}$	heat duty in device u in period t of operation [kW]
$TotalCost$	total cost [\$]
$TotalCostI$	total cost calculated with the maximum area for each heat transfer device [\$]

6. ACKNOWLEDGMENTS

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REFERENCES

- [1] Linnhoff, B., Kotjabasakis, E., (1986). Downstream paths for operable process design. *Chemical Engineering Progress*. 82:23-28.
- [2] Kotjabasakis, E., Linnhoff, B., (1986) Sensitivity tables for the design of flexible processes (1) – How much contingency in heat exchanger networks is cost-effective? *Chemical Engineering Research and Design*. 64:197-211.
- [3] Ravagnani, M. A. S. S., Módenes, A. N., (1996). Heat exchanger networks with multiple periods of operation. *Brazilian Journal of Chemical Engineering*. 13:71-84.
- [4] Floudas, C. A., Grossmann, I. E., (1986). Synthesis of flexible heat exchanger networks for multiperiod operation. *Comput. Chem. Eng.* 10, 2:153-168.
- [5] Papoulias, S. A., Grossmann, I. E., (1983). A structural optimization approach in process synthesis. Part II: Heat recovery networks. *Comput. Chem. Eng.* 7, 6:707-721.
- [6] Floudas, C. A., Grossmann, I. E., (1987a). Automatic generation of multiperiod heat

- exchanger network configuration. *Comput. Chem. Eng.* 11, 2:123-142.
- [7] Floudas, C. A., Ciric, A. R.; Grossmann, I. E., (1986). Automatic synthesis of optimum heat exchanger network configurations. *AIChE J.* 32, 2:276-290.
- [8] Aaltola, J., (2002). Simultaneous synthesis of flexible heat exchanger network. *Applied Thermal Engineering*. 22: 907-918.
- [9] Yee, T. F., Grossmann, I. E., (1990). Simultaneous optimization models for heat integration - II. Heat exchanger network synthesis. *Comput. Chem. Eng.*, 14: 1165-1184.
- [10] Verheyen, W.; Zhang, N., (2006). Design of flexible heat exchanger network for multi-period operation. *Chem. Eng. Sci.* 61:7730-7753.
- [11] Chen, C. L., Hung, P. S. (2007). Synthesis of flexible heat exchange networks and mass exchange networks. *Computers & Chemical Engineering*. 31: 1619-1632.
- [12] Chen, C. L., Hung, P. S., (2004). Simultaneous synthesis of flexible heat-exchange networks with uncertain source-stream temperatures and flow rates. *Ind. Eng. Chem. Res.* 43, 18:5916-5928.
- [13] Isafiade, A. J., Fraser, D. M., (2010). Interval based MINLP superstructure synthesis of heat exchanger networks for multi-period operations. *Chem. Eng. Res. Des.*, v. 88, p. 1329-1341.
- [14] Isafiade, A. J.; Fraser, D. M. (2008) Interval-based MINLP superstructure synthesis of heat exchanger networks. *Chem. Eng. Res. Des.* v. 86, p. 245-257.
- [15] Jiang, D., Chang, C. T., (2013). A New Approach to Generate Flexible Multiperiod Heat Exchanger Network Designs with Timesharing Mechanisms. *Ind. Eng. Chem. Res.* 52:3794-3804.
- [16] Nemet, A., Klemes, J. J., Kravanja, Z., (2013). Optimising entire lifetime economy of heat exchanger networks. *Energy*. 57: 222-235.

- [17] Li, J., Du, J., Zhao, Z., Yao, P., (2014). Structure and area optimization of flexible heat exchanger networks. *Industrial & Engineering Chemistry Research*. 53:11779-11793.
- [18] Isafiade, A., Bogataj, M., Fraser, D., Kravanja, Z., (2015). Optimal synthesis of heat exchanger networks for multi-period operations involving single and multiple utilities. *Chem. Eng. Sci.*, v. 127, p. 175-188.
- [19] El-Temtamy, S. A., Gabr, E. M., (2012). Design of optimum flexible heat exchanger networks for multiperiod process. *Egyptian Journal of Petroleum*. 21:109-117.
- [20] Mian, A., Martelli, E., Maréchal, F., (2016). Framework for the Multiperiod Sequential Synthesis of Heat Exchanger Networks with Selection, Design, and Scheduling of Multiple Utilities. *Ind. Eng. Chem. Res.*, 55, 168-186.
- [21] Ma, X., Yao, P., Luo, X., Roetzel, W., (2008). Synthesis of multi-stream heat exchanger network for multi-period operation with genetic/simulated annealing algorithms. *Applied Thermal Engineering*. 28: 809-823.
- [22] Ahmad, M. I., Zhang, N., Jobson, M., Chen, L., (2012). Multi-period design of heat exchanger networks. *Chemical Engineering Research and Design*. 90:1883-1895.
- [23] Yi, D., Han, Z., Wang, K., Yao, P., (2013). Strategy for synthesis of flexible heat exchanger networks embedded with system reliability analysis. *Chinese Journal of Chemical Engineering*. 21, 7: 742-753.
- [24] Chen, J. J. J., (1987). Letters to the editors: comments on improvements on a replacement for the logarithmic mean. *Chem. Eng. Sci.* 42, 10:2488-2489.
- [25] Floudas, C. A., Grossmann, I. E., (1987b). Synthesis of flexible heat exchanger networks with uncertain flowrates and temperatures. *Comput. Chem. Eng.* 11, 4:319-336.

Figure Captions

Figure 1: Diagram summarizing methodology steps

Figure 2: Multiperiod superstructure for a hot stream

Figure 3: Streams and sub-networks for Example 1.

Figure 4: Final HEN structure for Example 1. Presented values are hot streams temperatures in °C in each period.

Figure 5: Final HEN for Example 1 with detailed information on heat capacities and streams temperature in each point of the network in each period

Figure 6: Final HEN structure for Example 2. Presented values are hot streams temperatures in K in each period.

Figure 7: Final HEN for Example 2 with detailed information on heat capacities and streams temperature in each point of the network in each period

Figure 8: Final HEN presented by Isafiade and Fraser [13] for Example 2.

Table 1: Example 1 data

Stream	T_{in} (°C)	T_{out} (°C)	F (kW/°C)
Period 1			
H1	249.0	100.0	10.550
H2	259.0	128.0	12.660
C1	96.0	170.0	9.144
C2	106.0	270.0	15.000
Period 2			
H1	229.0	120.0	7.032
H2	239.0	148.0	8.440
C1	96.0	170.0	9.144
C2	106.0	270.0	15.000
Period 3			
H1	249.0	100.0	10.550
H2	259.0	128.0	12.660
C1	116.0	150.0	6.096
C2	126.0	250.0	10.000

Table 2: Minimum utilities demand and pinch point in the different periods of Example 1

	QS_m (kW)	QW_n (kW)	Pinch Point temperature ($^{\circ}\text{C}$)
Period 1	338.40	432.15	249.0 – 239.0
Period 2	1602.13	0.00	-----
Period 3	10.00	1793.15	259.0 – 249.0

Table 3: Matches and heat duties (kW) for each period of Example 1

Device	Match	Period 1	Period 2	Period 3
U1	HU-C2	338.40	1602.13	10.00 *
U2	H2-C2	126.60	0.00	0.00
U3	H1-C1	676.66	676.66	207.26
U4	H1-C2	817.93	89.83	1045.85
U5	H2-C2	1177.07	768.04	184.15
U6	H1-CU	77.36	0.00	318.84
U7	H2-CU	354.79	0.00	1474.31

* The line indicates sub-networks division

Table 4: Individual areas and global heat transfer coefficients for each match and cost data for Example 1

Device	Match	Co_u (kW/m ² °C)	AreaM (m ²)
U1	HU-C2	0.8	28.76
U2	H2-C2	1.0	11.79
U3	H1-C1	1.0	28.19
U4	H1-C2	1.0	84.88
U5	H2-C2	1.0	57.97
U6	H1-CU	0.4	10.63
U7	H2-CU	0.3	34.92

$$Cost = 4333 \cdot Area^{0.6}, Area [=] m^2.$$

Hot utility cost (300-300 °C) = 171.428×10^{-4} \$/kWh.

Cold utility cost (30-50 °C) = 60.576×10^{-4} \$/kWh.

Annualizing factor = 0.2

Table 5: Comparison among costs found in this study and findings published previously in the literature for Example 1

	Utilities cost (\$/h)			Capital cost (\$)
	Period 1	Period 2	Period 3	
Floudas and Grossmann [6]	8.418	27.465	11.033	269,380.00
Isafiade and Fraser [13]	44.411	36.696	28.747	134,774.39
Isafiade et al. [18]	73.340	63.060	44.380	125,371.07
Mian et al. [20]	-----*	-----*	-----*	235,160.00
This study	8.418	27.465	11.033	249,845.93

* Values not reported by the authors.

Table 6: Comparison among annualized cost found in this study and findings published previously in the literature for Example 1 (\$/year)

	Utility cost	Capital cost	Total cost
Floudas and Grossmann [6]	134,492	53,876	188,368
Isafiade and Fraser [13]	314,731	26,926	341,657
Isafiade et al. [18]	518,236	24,263	542,499
Mian et al. [20]	138,660	47,032	185,692
This study	134,492	49,969	184,461

Table 7: Example 2 data

Stream	T_{in} (K)	T_{out} (K)	F (kW/K)
Nominal conditions			
H1	583.0	323.0	1.400
H2	723.0	553.0	2.000
C1	313.0	393.0	3.000
C2	388.0	553.0	2.000
HU	573.0	573.0	--
CU	303.0	323.0	--
Period 1			
H1	593.0	323.0	1.800
H2	723.0	553.0	2.000
C1	313.0	393.0	3.000
C2	383.0	553.0	2.400
Period 2			
H1	593.0	323.0	1.800
H2	723.0	553.0	2.000
C1	313.0	393.0	3.000
C2	393.0	553.0	1.600
Period 3			
H1	573.0	323.0	1.000
H2	723.0	553.0	2.000
C1	313.0	393.0	3.000
C2	383.0	553.0	2.400

Table 8: Minimum utilities demand and pinch point in the different periods of Example 2

	QS_m (kW)	QW_n (kW)	Pinch Point (K)
Nominal conditions	0	134	----
Period 1	0	178	----
Period 2	0	330	----
Period 3	68	10	333.0 – 313.0

Table 9: Matches and heat duties (kW) for each period of Example 2

Device	Match	Nominal conditions	Period 1	Period 2	Period 3
U1	HU-C1	0	0	0	68
U2	H1-C1	180	240	156	142
U3	H1-C2	50	68	0	98
U4	H2-C1	60	0	84	30
U5	H2-C2	280	340	256	310 *
U6	H1-CU	134	178	330	10

* This line indicates the sub-networks division

Table 10: Individual areas and global heat transfer coefficients for each match and cost data for Example 2.

Device	Match	Co_u (kW/m ² K)	AreaM (m ²)
U1	HU-C1	0.08	4.46
U2	H1-C1	0.08	33.08
U3	H1-C2	0.08	10.36
U4	H2-C1	0.08	3.71
U5	H2-C2	0.08	26.07
U6	H1-CU	0.08	57.32

$$Cost = 4333 \cdot Area^{0.6}, Area [=] m^2.$$

$$\text{Steam cost (573-573 K)} = 171.428 \times 10^{-4} \text{ \$/kWh.}$$

$$\text{Cooling water cost (303-323 K)} = 60.576 \times 10^{-4} \text{ \$/kWh.}$$

$$\text{Annualizing factor} = 0.2$$

Table 11: Utility, capital and annualized cost of the HEN found in this study for Example

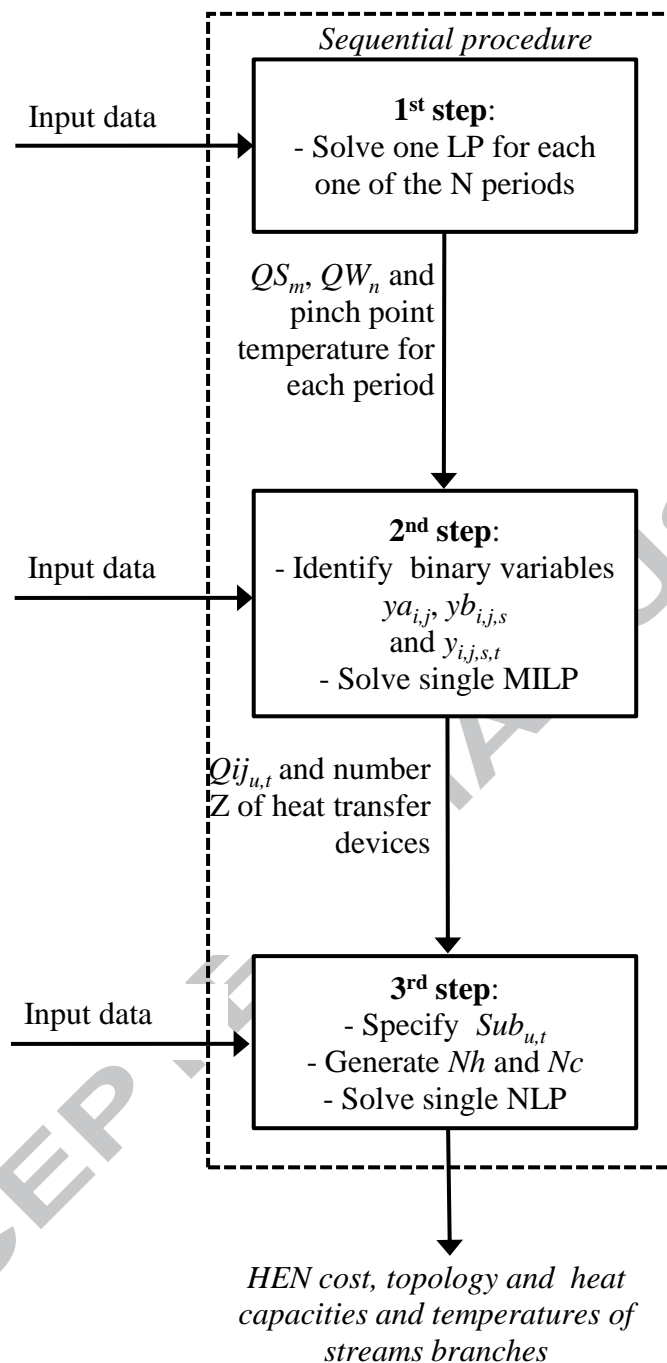
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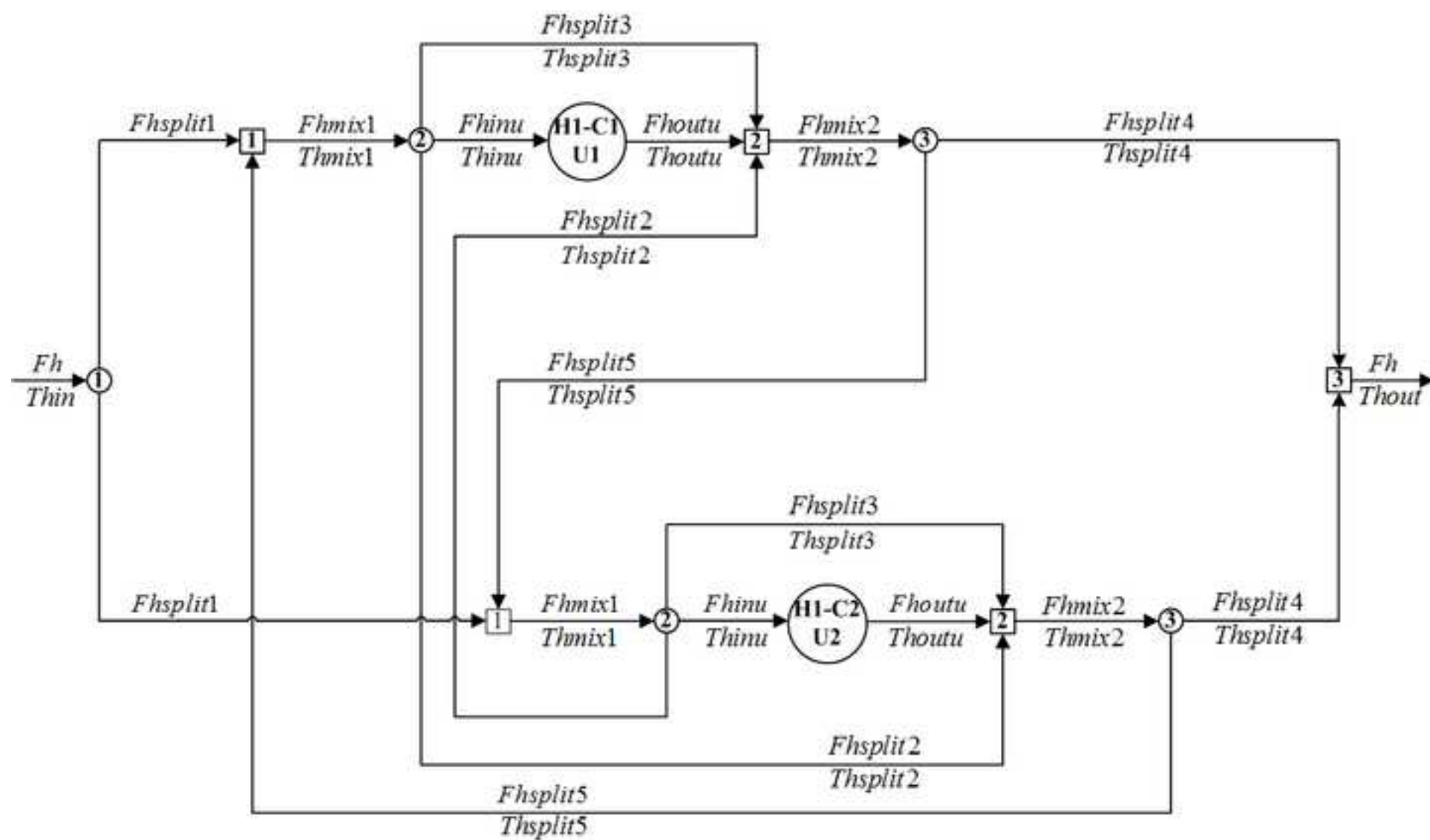
		Individual costs	Annualized costs
Utility cost	Nominal conditions	\$ 0.8117 / h	\$ 1,745.15 / yr
	Period 1	\$ 1.0782 / h	\$ 2,318.13 / yr
	Period 2	\$ 1.9990 / h	\$ 4,297.85 / yr
	Period 3	\$ 1.2263 / h	\$ 2,636.54 / yr
Capital cost		\$ 152,956.94	\$ 30,591.39 / yr

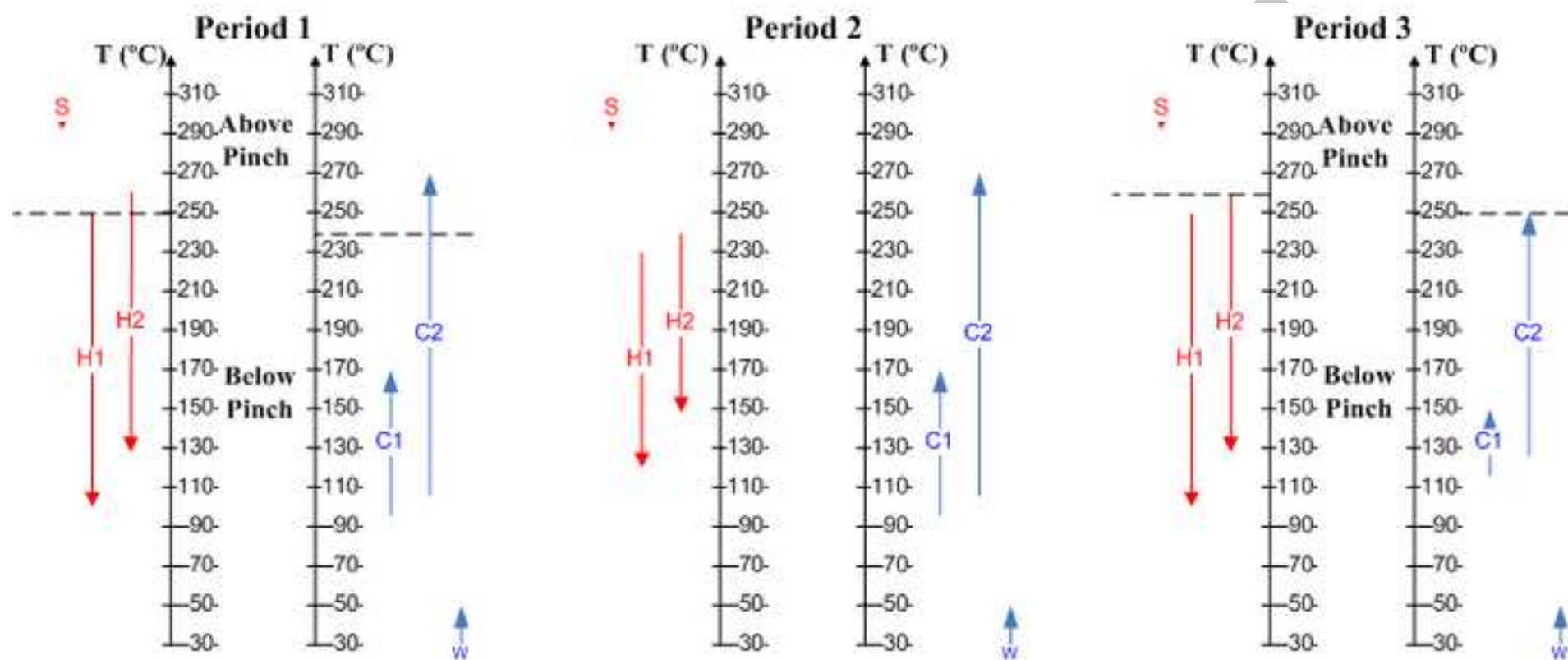
Table 12: Comparison among annualized cost found in this study and findings published previously in the literature for Example 2 (\$/year)

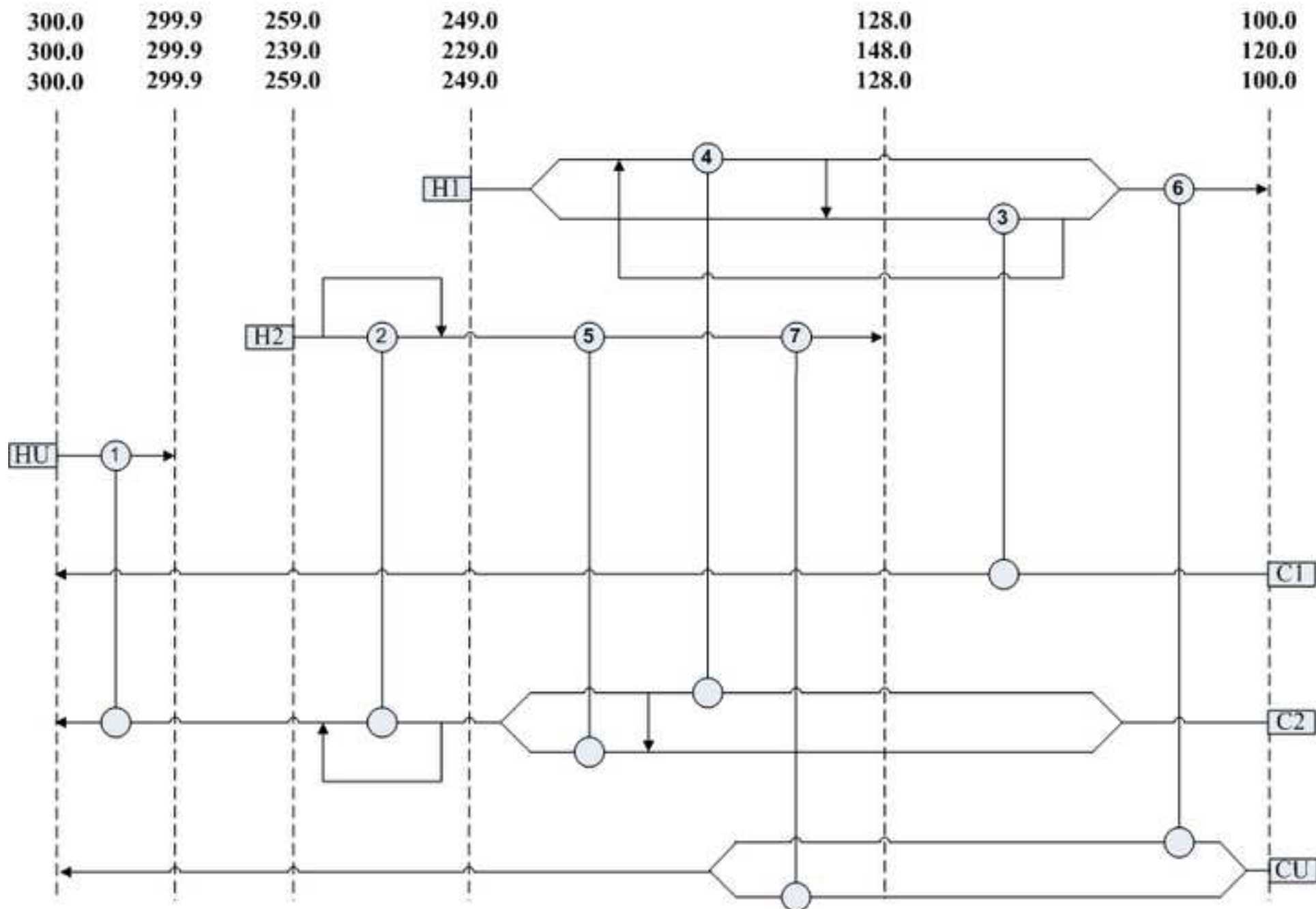
	Total cost (\$/yr)
Floudas and Grossmann [25]	49,879
Chen and Hung [12]	41,876
Isafiade and Fraser [13]	39,660
This study	41,589

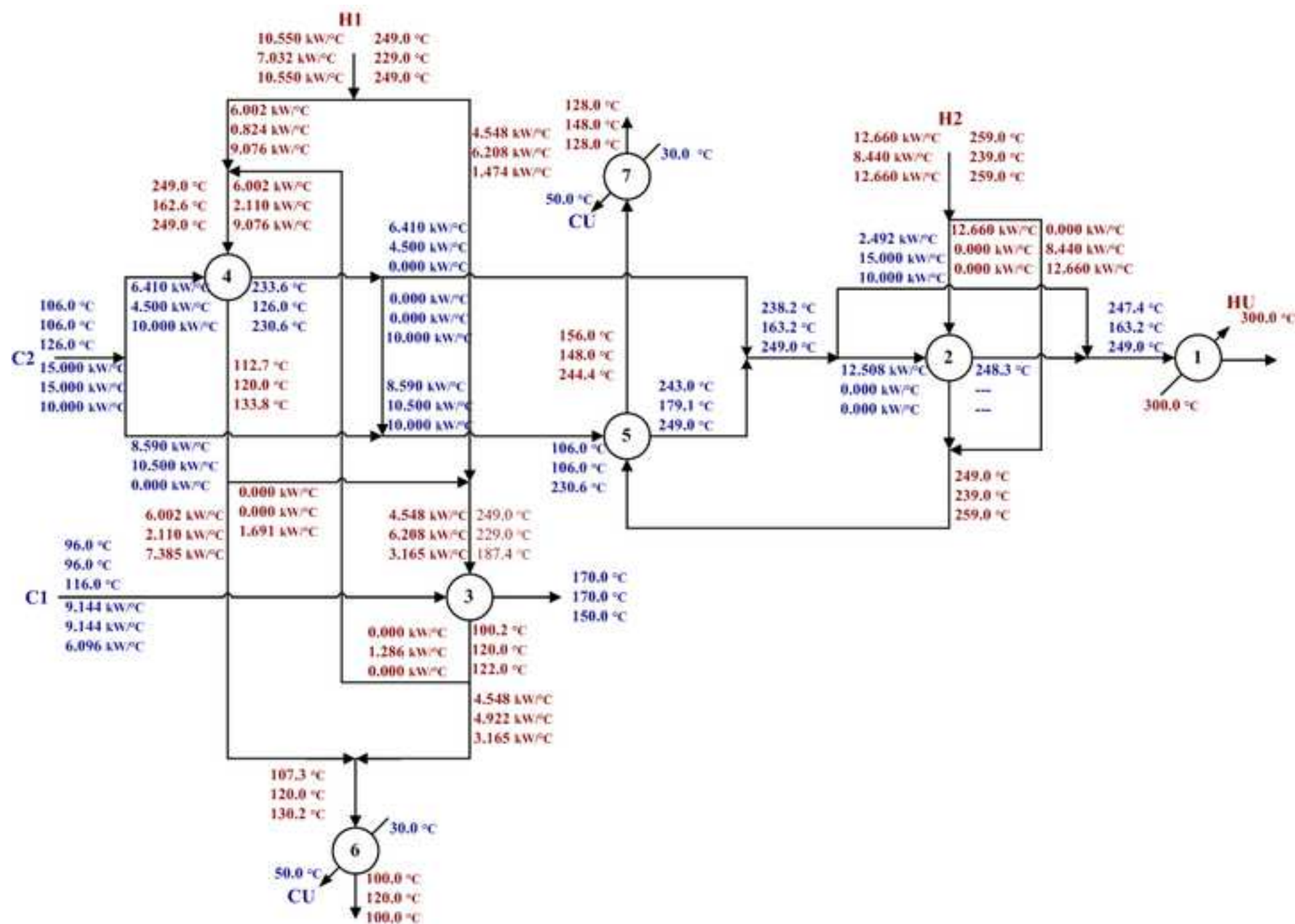
Figure 1

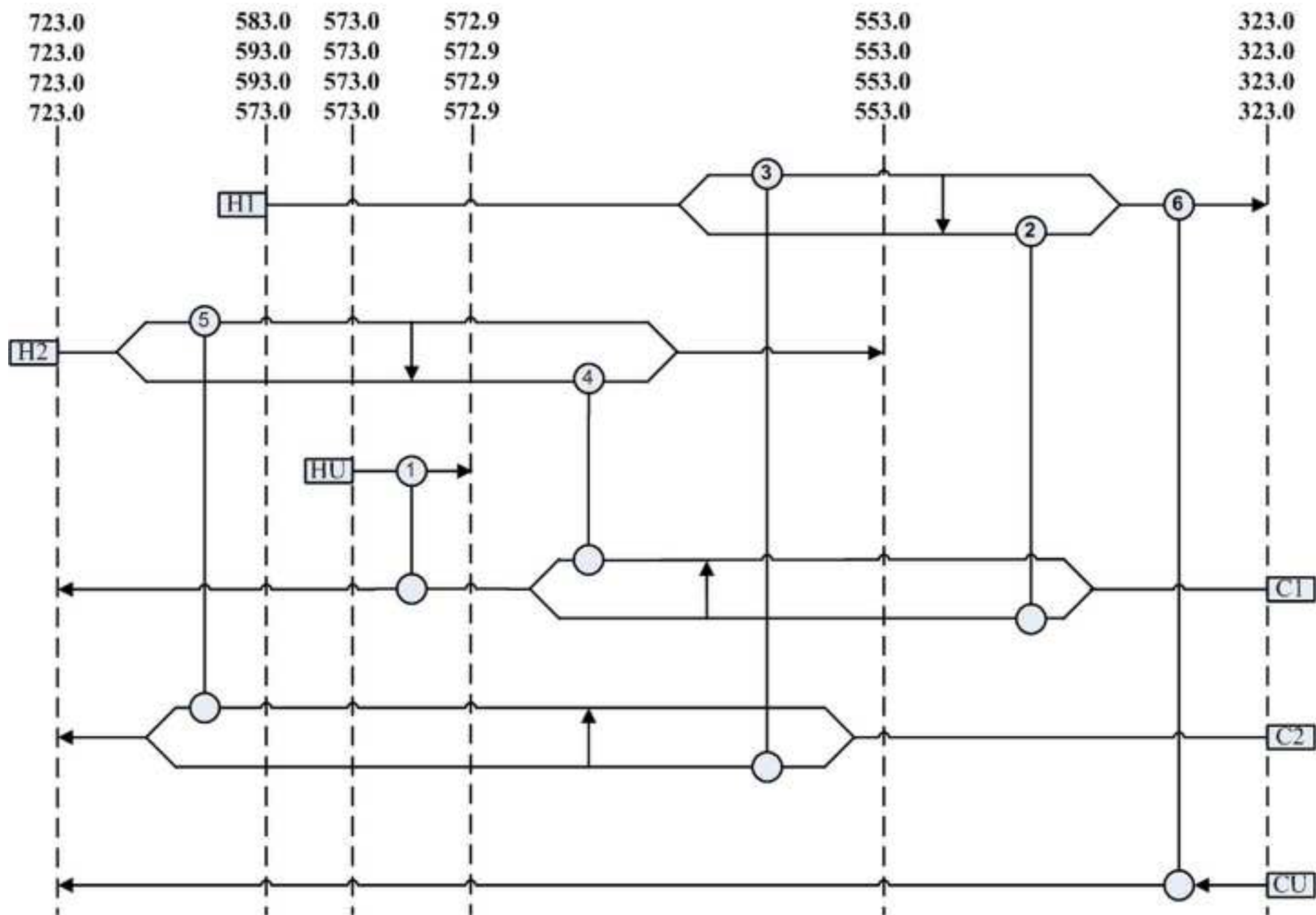


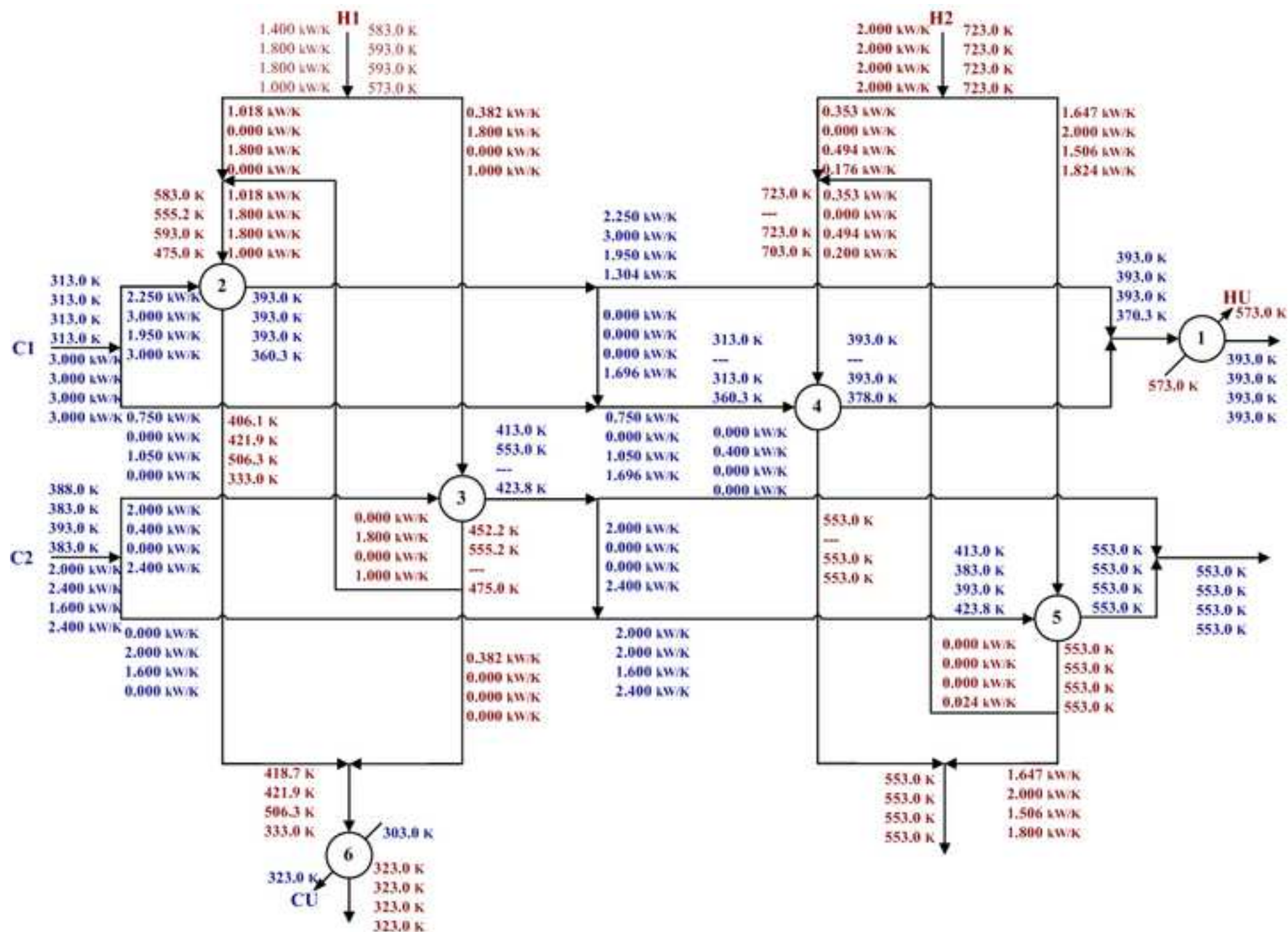


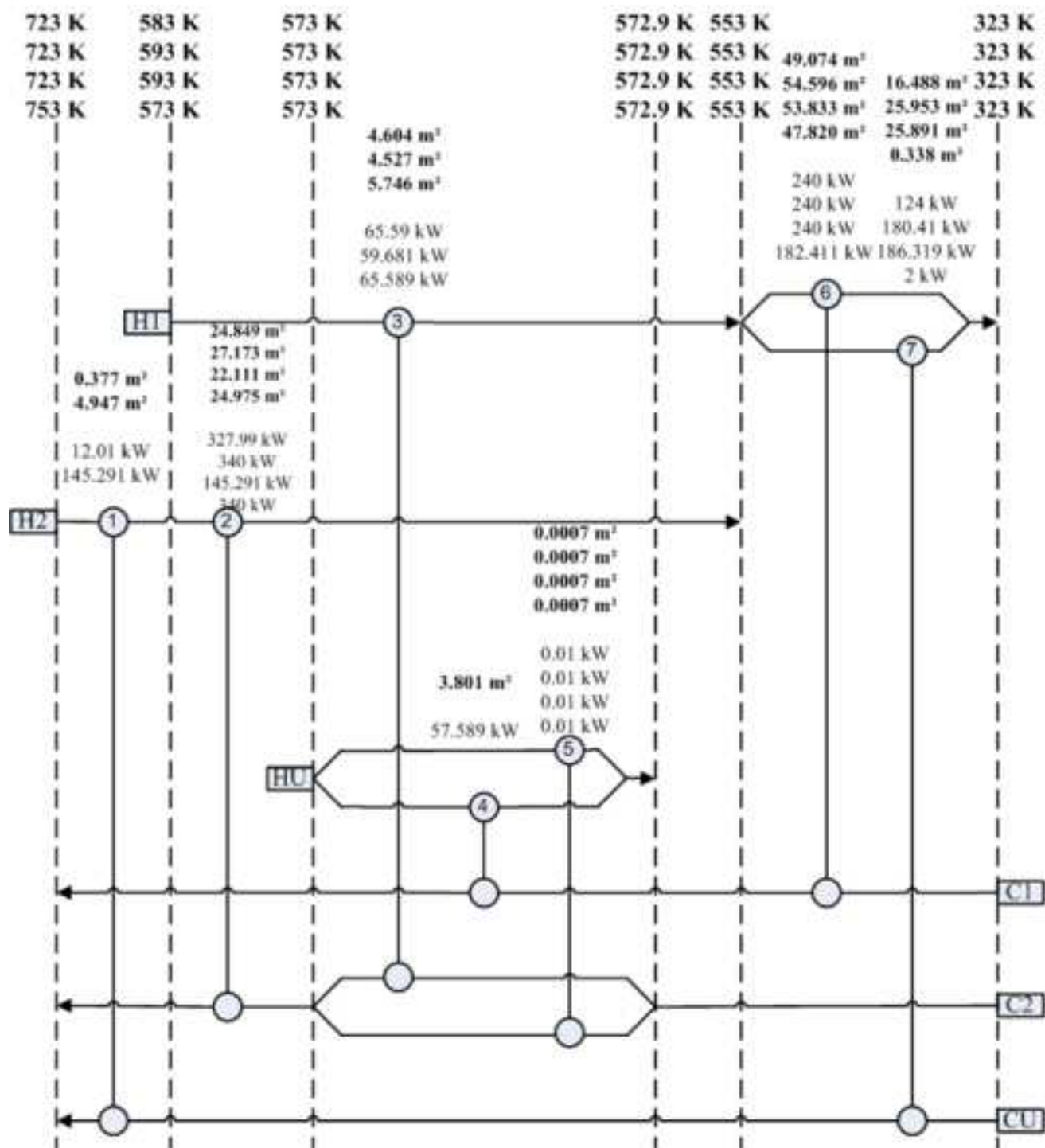












Highlights

- A sequential approach for the synthesis of multiperiod HEN is provided.
- A well-known superstructure was improved.
- Two sets and one parameter were created to decrease the NLP model complexity.
- NLP model for the capital cost evaluation was modified.
- Better results for literature problems were found by applying the model.